Information entropy and the study of atoms in the quantum world

Student: Christos Pilitsidis

Course: Computational Quantum Physics

Professor: K.Chatzisavvas

July 2025

Contents

1) Introduction/Theory

In the last few decades the interest for the information properties of quantum mechanical systems has increased. The **information properties of quantum mechanical systems** have become a central topic in modern physics, chemistry, and even quantum computing. People study information properties of quantum systems to better understand **the structure and behavior** of atoms, molecules, and quantum fields and to improve quantum technologies.

Quantum mechanics is fundamentally **probabilistic**, not deterministic. Information-theoretic tools help answer questions like:

- *How much uncertainty is there in a quantum state?*
- *How "spread out" or localized is an electron in an atom or molecule?*

This is studied using measures like **Shannon entropy**, **Fisher information**, and **Rényi entropy.**

The aim of this project is to study the information content of **the first 10 atoms multi-electron** of the periodic table(excluding Hydrogen). To achieve this, we carry out a study of the **Shannon entropy** in position and momentum space, and also we compute other quantities to understand better atoms.

To calculate essentially any type of quantity in the quantum world, we need a probability distribution as the notion of definite position of particles(or momentum) no longer is valid. The only way to attain the probability distribution is from solving the Schrödinger equation for a multi-electron system to get the wave-function. However, this is a very difficult task and impossible to solve analytically.

We applied the Roothaan-Hartree-Fock method to calculate analytical self-consistent-field atomic wave functions. Self-consistent means we start with a guess for the wavefunction and then compute a mean-potential from the Schrödinger equation. Then for this potential we solve the same equation and get another output wavefunction. We repeat the process untill the intial and the output wavefunction differ a little. That's what it means self-consistent.

Also, we made two important assumptions. The first one is the electrons do not interact with each other and they only 'see' an average field of the nucleus and of the other electrons. And the second assumption is that we have spherical symmetry in the solutions-wavefunctions.

In the Roothaan-Hartree-Fock approach, the radial atomic wavefunctions $R_{nl}(r)$ are expanded as a finite superposition of primitive radial functions:

$$R_{nl}(r) = \Sigma_j\ C_{jnl}\ S_{jl}(r)$$

where the normalized primitive basis $S_{jl}(r)$ is taken as a Slater-type orbital set:

$$S_{jl}(r) = N_{jl} \cdot r^{n_{jl}-1} \cdot \exp(-Z_{jl} \cdot r)$$

The normalization factor N_{jl} is given by:

$$N_{jl} = [\ (2Z_{jl})^{(2n_{jl})} / (2n_{jl})!\ ]^{1/2}$$

where n_{jl} is the principal quantum number and Z_{jl} is the orbital exponent.

After knowing the radial wavefunctions we can take the square of them and take an appropriate linear combination of them(depends on the element and the atomic orbitals it has) to get the probability distribution pr. Then we can compute quantities like the Shannon entropy:

$$\mathbf{Sr} = -\int \rho(r)\ln\rho(r)dr \quad \text{or in } \mathbf{k\text{-}space} \quad \mathbf{Sk} = -\int n(k)\ln n(k)dk$$

Where **n(k)** can be calculated by a **Fourier transform** from **ρ(r)**.

For all the calculations i used the mathematica software and for every element from He(Z=2) till Ne(Z=10) i created a separate notebook. I used the coefficients and numbers to get the wavefunctions for each orbital from the table [1]. The final useful data that i got from all these calculations i inserted in a notebook plots.nb where i created the required plots.

The Mathematica software is dynamic, so variables and quantities from one notebook i can use in another one.

2) Plots and comments about them

The graph of entropy with respect to position space and k-space is shown below.
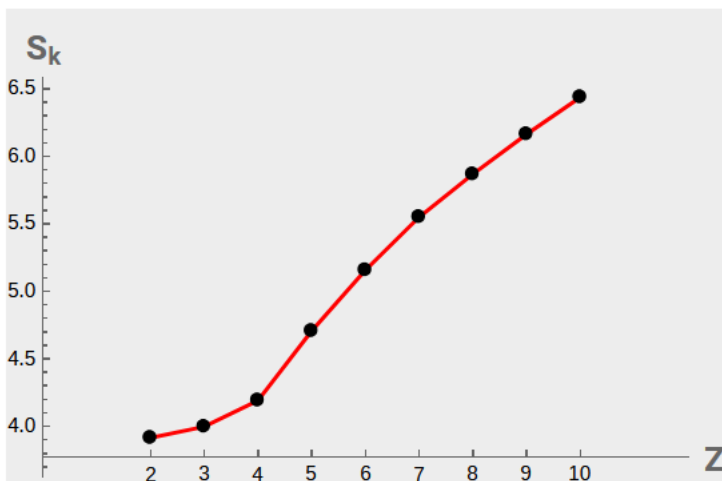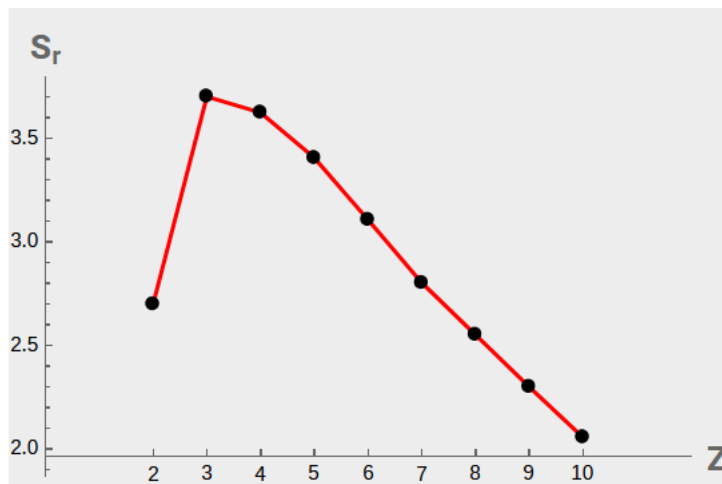

The fact that entropy in position space decreases with Z means that for bigger atoms of the periodic table we expect more order. The opposite is true in k-space were we expect more complexity and less order.

The total Shannon entropy is shown below. It follows a steady increasing trend, which is not linear. Below, the maximum value of entropy is depicted. From He to Li it increases and then steadily decreases as the entropy in position space does.
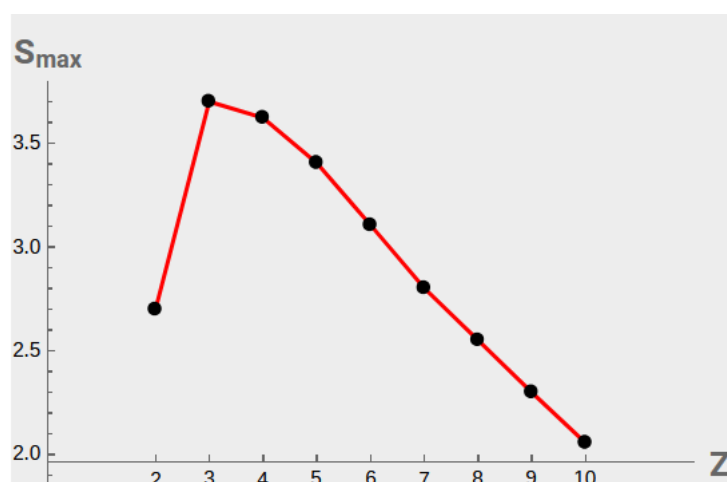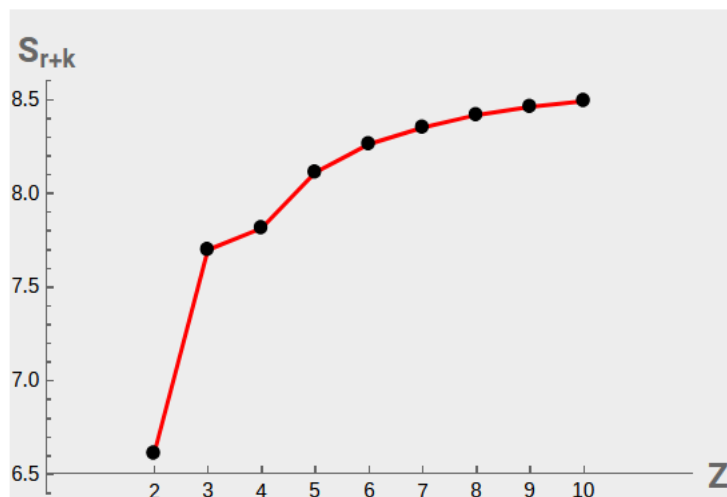
Finally the Landsberg parameter Ω and the dimensionless quantity O are shown. O is the inverse of the product of Onicescu entropies in position and k-space. It measures the complexity of the system as a whole. From the graph below, O reduces after Li as Z increases which reflects that the distributions in both spaces are not localized overall.
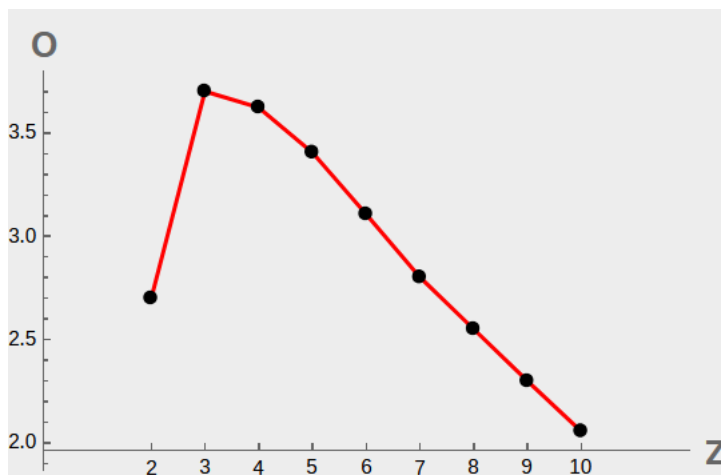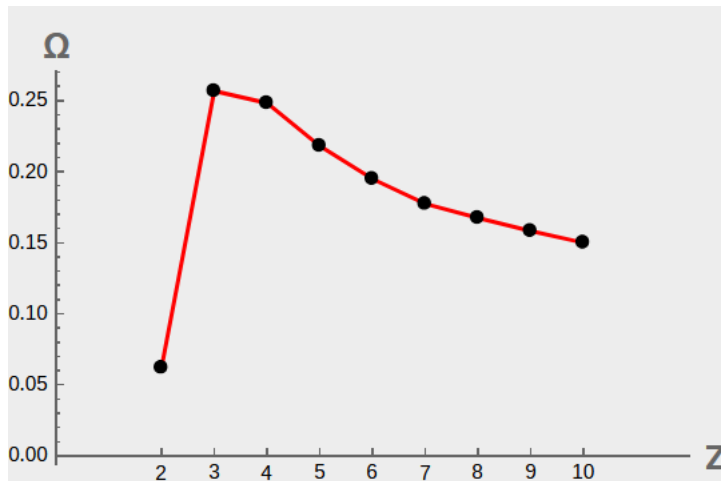
3) Extra task-Relation Z and S

From the previous graph of S total entropy and Z atomic number, we can conclude that S and Z are not linearly dependent. From the paper [2] we see in page 5,on Figure 2 that S is logarithmically dependent on Z approximately **S=6.257+1.069lnZ.**

After some algebraic manipulation we can write Z as a function of S like this:

Z = a · exp(bS) where a,b are constants that need to be found.

In the notebook BonusExercise.nb i calculate them and i plot the figure that follows.
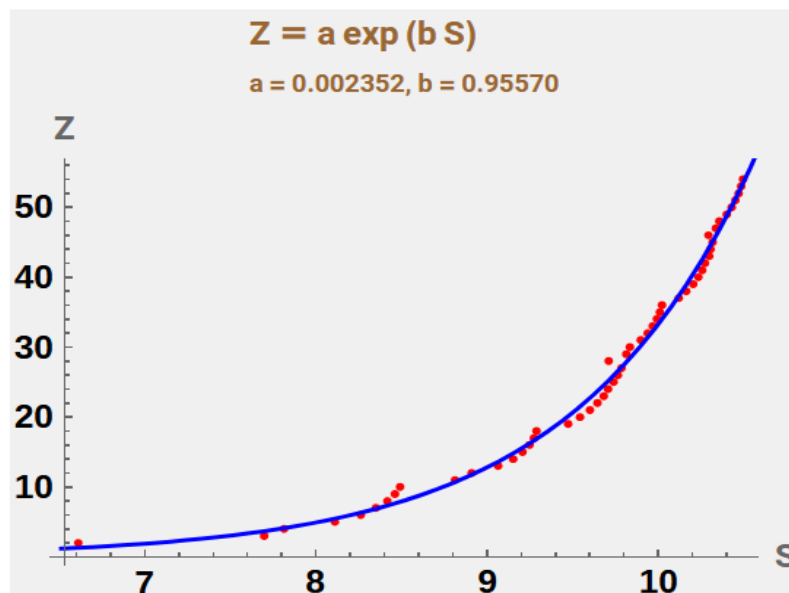
The numerical values of a and b are shown in the figure. As we can observe, the non-linear regression model is very satisfactory-datapoints are very close to the blue curve of the exponential model.

5) References

[1] F.Bunge, J.A.Barrientos and A.V.Bunge, 162 At.Data Nucl. Data Tables 53,113 (1993)

[2] K.Ch.Chatzisavvas, Ch.Moustakidis and C.P.Panos, Journal of Chem.Phys. 123,174111(2005)